Corrections to scaling for block entanglement in massive spin-chains

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Abstract. We consider the Rényi entropies S_n in one-dimensional massive integrable models diagonalizable by means of corner transfer matrices (as Heisenberg and Ising spin chains). By means of explicit examples and using the relation of corner transfer matrix with the Virasoro algebra, we show that close to a conformal invariant critical point, when the correlation length ξ is finite but large, the corrections to the scaling are of the *unusual* form $\xi^{-x/n}$, with x the dimension of a relevant operator in the conformal theory. This is reminiscent of the results for gapless chains and should be valid for any massive one-dimensional model close to a conformal critical point.

1. Introduction

In the last decade there has been an increasing interest in quantifying the amount of entanglement that is present in the ground state of an extended quantum system [1]. A measure of the bipartite entanglement is given by the so-called Rényi entropies, defined as follows. Let $|\Psi\rangle$ be the ground state of an extended quantum mechanical system and $\rho = |\Psi\rangle\langle\Psi|$ its density matrix. One then divides the Hilbert space into a part $\mathcal{A}$ and its complement $\mathcal{B}$ and considers the reduced density matrix $\rho_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}}\,\rho$ of subsystem $\mathcal{A}$. Finally, the Rényi entropies are given by

$$S_n = \frac{1}{1-n} \ln \mathrm{Tr}\, \rho_{\mathcal{A}}^n \,. \tag{1}$$

The particular case $n = 1$ of (1) is the von Neumann entropy S_1 and it is usually called simply *entanglement entropy*. However, the knowledge of S_n for different n characterizes the full spectrum of non-zero eigenvalues of $\rho_{\mathcal{A}}$ (see e.g. [2]) and provides significantly more information than S_1.

The case that has been most widely studied is a critical one-dimensional system whose continuum limit is described by a conformal field theory (CFT) of central charge c. When $\mathcal{A}$ is an interval of length ℓ embedded in an infinite system, the asymptotic large-ℓ behavior of the Rényi entropies is given by [3, 4, 5]

$$S_n(\ell) \simeq \frac{c}{6}\left(1+\frac{1}{n}\right)\ln\ell + c'_n \,, \tag{2}$$

where c'_n is a non-universal constant. This behavior has been verified analytically and numerically in numerous models. Only more recently it has been realized that such asymptotic behavior can be difficult to observe because of the presence of large and *unusual* corrections to the scaling behaving like [6, 7, 8]

$$S_n(\ell) \simeq \frac{c}{6}\left(1+\frac{1}{n}\right)\ln\ell + c'_n + b_n \ell^{-2x/n} \,, \tag{3}$$

where x is the scaling dimension of a relevant operator (i.e. $x < 2$) and b_n another non-universal constant. These power-law corrections decay slowly even for moderate values of n and completely obscure the asymptotic result for large n. In field theory language, this unusual scaling originates from the conical singularities (at the boundary between $\mathcal{A}$ and $\mathcal{B}$) present in the n-sheeted Riemann surface describing $\mathrm{Tr}\rho_{\mathcal{A}}^n$ [7].

However, universal scaling is not a prerogative of the gapless models. A nearby critical point influences a part of the parameter space called 'critical region' in which the correlation length ξ (inverse gap) is large but finite. Simple scaling arguments suggest that when an infinite system is divided in two semi-infinite halves, the entanglement entropy should scale as

$$S_n \simeq \frac{c}{12}\left(1+\frac{1}{n}\right)\ln\xi + C'_n \,, \tag{4}$$

where C'_n is yet another non-universal constant. (One could also fix the normalization of the correlation length in such a way that $C'_n = c'_n/2$ as done in some practical instances [9].) This formula has indeed been corroborated by a general field-theory argument that parallels the c-theorem [4] and it has been verified for many integrable models. In this massive case, the spatial division in $\mathcal{A}$ and $\mathcal{B}$ is not as important as in the massless case. Indeed as long as the correlation length is smaller than all the separations (e.g. ℓ above), the Rényi entropies of many disjoint blocks are given

by Eq. (4) multiplied by the number of boundary points between $\mathcal{A}$ and $\mathcal{B}$. This is nothing but the one-dimensional area law. The question that naturally arises is whether *unusual* corrections to the scaling in ξ would be also present for the massive case. By simple scaling hypothesis, one could argue that corrections due to a finite correlation length in Eq. (3) should be functions of ξ/ℓ and then changing the limit from $\ell \ll \xi$ to $\ell \gg \xi$, one argues

$$S_n \simeq \frac{c}{12}\left(1+\frac{1}{n}\right)\ln\xi + C'_n + B_n \xi^{-x/n}\,. \tag{5}$$

(Notice that the exponent of the corrections is half the one in (3) because of the presence of a single conical singularity, analogously to the case of critical systems with boundaries [7]). However, because of the very unusual form of these corrections, one could doubt whether such a simple scaling argument gives the correct answer.‡ Here we provide the analytical evidence that in some integrable models in which S_n can be obtained through the Baxter corner transfer matrix [10] this scaling is indeed correct and that further corrections are of the form $\xi^{-kx/n}$ and ξ^{-kx} with k integer.

2. Corrections to the scaling of Rényi entropies using corner transfer matrix

When dealing with the geometric bipartition considered in this paper (i.e. two semi-infinite half lines) the corner transfer matrix (CTM)– that is a classical tool of statistical mechanics [10]– helps considerably in the derivation of the reduced density matrix $\rho_{\mathcal{A}}$ and hence for the characterization of the entanglement entropies [4, 11].

In two-dimensional statistical models the CTM $\hat{A}$ is the transfer matrix that connects an horizontal row (let say the line $x<0$) to a vertical one (let say $y<0$). Rigorously speaking, each element of $\hat{A}$ is the partition function of the left-lower quadrant when the spins on the negative x and y axes are fixed to given values. If, following Baxter [10], we choose the lattice in a clever way (i.e. rotated by $\pi/4$ with respect to the axes), the four corner transfer matrices are all equivalent (under some symmetry requirements on the model) and the full partition function is just $\mathrm{Tr}\hat{A}^4$. It is also evident that the reduced density matrix of the quantum problem whose time-discretized version is the classical model under consideration (see e.g [12, 13]) is

$$\rho_{\mathcal{A}} = \frac{\hat{A}^4}{\mathrm{Tr}\hat{A}^4}\,, \tag{6}$$

where the denominator is fixed by the normalization $\mathrm{Tr}\rho_{\mathcal{A}} = 1$.

For several models, it is possible to obtain this reduced density matrix exactly in the infinite-lattice limit.. It always assumes the form [13, 11]

$$\rho_{\mathcal{A}} = \frac{e^{-H_{\mathrm{CTM}}}}{\mathrm{Tr}\, e^{-H_{\mathrm{CTM}}}}\,, \tag{7}$$

where $\hat{H}_{\mathrm{CTM}}$ is an effective Hamiltonian, which, for many interesting integrable massive models, may be rewritten in terms of free-fermionic operators (see [13] and references therein)

$$H_{\mathrm{CTM}} = \sum_{j=0}^{\infty} \epsilon_j n_j\,. \tag{8}$$

‡ This scaling analysis is corroborated by recent results for gapless systems in a trapping potential [9]. In this case, the actual system is gapless, but a length scale is generated by the trapping potential and the resulting scaling is exactly given by Eq. (5) where ξ is replaced by the trap-scale.

where $n_j = c_i^\dagger c_i$ are fermion occupation numbers and have eigenvalues 0 and 1. These properties are very general features of a large class of massive integrable spin-chains. The specificity of the model comes from the functional form of the "single-particle levels" ϵ_j. In this basis $\rho_{\mathcal{A}}$ is diagonal and so the Rényi entropies are easily written for any value of n, not only integer.

One should mention that, for a given lattice Hamiltonian, there are several ways to construct a CTM. The one used above is particularly convenient because then the RDM is just its fourth power. In general, ρ_A will be given by the product 'ABCD' of four different CTMs which also not need to be symmetric (although the product is). CTMs can be defined also for non-integrable models, but then one does not have closed and simple formulae for the eigenvalues and has to work numerically, see e.g. Ref. [12].

2.1. Non-critical XXZ chain

We start our analysis from the anisotropic Heisenberg model with Hamiltonian

$$H_{XXZ} = \sum_j \left[\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z\right] , \tag{9}$$

where σ's are the Pauli matrices. This model is gapless for $|\Delta| \leq 1$ and gapped for $|\Delta| > 1$ with a conformal point at $\Delta = 1$. We study the antiferromagnetic gapped regime with $\Delta > 1$. The XXZ model is usually solved by Bethe ansatz that is the most suited framework to calculate thermodynamical properties as well as correlation functions. Unfortunately, Bethe ansatz is still rather ineffective to provide the entanglement entropies both in the coordinate [14] and algebraic [15] approaches. Also the special combinatoric features at $\Delta = 1/2$ only allowed the calculation of S_n up to $\ell = 6$ [16]. By contrast, the CTM solution is very simple and the "single-particle levels" of the resulting $H_{\rm CTM}$ are exactly known [13]

$$\epsilon_j = 2j\epsilon \qquad \text{with} \qquad \epsilon = \text{arccosh}\Delta\,. \tag{10}$$

The correlation length of the model is also exactly known as function of Δ [10], but for what follows we are only interested in its universal part in the critical regime $\xi \gg 1$

$$\ln \xi \simeq \frac{\pi^2}{2\epsilon} + O(\epsilon^0)\,. \tag{11}$$

The Rényi entropies are written straightforwardly§

$$S_n = \frac{1}{1-n}\left[\sum_{j=0}^{\infty} \log(1+e^{-2nj\epsilon}) - n\sum_{j=0}^{\infty} \log(1+e^{-2j\epsilon})\right] . \tag{12}$$

This formula is exact, but does not directly allow an expansion in terms of powers of the correlation length, i.e. for small ϵ. One could be tempted to perform an Euler Mac-Laurin summation, that gives the correct leading behavior [4]. Unfortunately the subleading corrections we are interested in are of the form $\xi^{-\alpha} \propto e^{-\alpha\pi^2/2\epsilon}$, that

§ Eq. (12) has already been derived (actually the double of it) for the XY spin chain by Franchini et al. in [17] by using previous results [18] based on integrable Fredholm operators and Riemann-Hilbert problem. It turns out that in the XXZ model, only the dependence of ϵ on the Hamiltonian parameters is different, but Eq. (12) is identical. This could not have been known a-priori. Deriving this result with CTM methods allows to generalize the treatment to other models (as the XXZ spin-chain) for which the Riemann-Hilbert problem is not known. In Ref. [17] S_n has been rewritten in terms of elliptic functions, while here we use a different strategy.

are not obtainable by the asymptotic expansion in power of ϵ^{-1} given by the Euler Mac-Laurin formula. One can however check straightforwardly that all the analytic corrections in ϵ indeed vanish (this has been observed in [19] for $n \to \infty$).

We obtain the truly asymptotic expansion for small ϵ by using the Poisson resummation formula (as similarly done for S_1 in [20]). This formula tells us that

$$\sum_{j=-\infty}^{\infty} f(|\epsilon j|) = \frac{2}{\epsilon} \sum_{k=-\infty}^{\infty} \hat{f}\left(\frac{2\pi k}{\epsilon}\right) , \tag{13}$$

where

$$\hat{f}(y) = \int_0^\infty f(x) \cos(yx) dx \,. \tag{14}$$

For Eq. (12), denoting with

$$f_n(x) = \log(1 + e^{-2nx}) \,, \tag{15}$$

we can rewrite the sum as

$$S_n = \frac{1}{1-n} \sum_{j=0}^{\infty} (f_n(\epsilon j) - n f_1(\epsilon j)) = \frac{1}{2} \frac{1}{1-n} \sum_{j=-\infty}^{\infty} (f_n(|\epsilon j|) - n f_1(|\epsilon j|)) + \frac{\ln 2}{2} \,, \tag{16}$$

where we used $f_n(0) = \ln 2$. The cosine-Fourier transform of $f_n(x)$ is

$$\hat{f}_n(y) = \frac{n}{y^2} - \frac{\pi}{2y} \text{csch} \frac{\pi x}{2n} \,, \tag{17}$$

Plugging the last equation in the Poisson resummation formula we have that the two terms n/y^2 simplify, leading to the compact result

$$S_n = \frac{1}{1-n} \sum_{k=-\infty}^{\infty} \left[\frac{n}{4k} \text{csch} \frac{\pi^2 k}{\epsilon} - \frac{1}{4k} \text{csch} \frac{\pi^2 k}{\epsilon n} \right] + \frac{\ln 2}{2} \,. \tag{18}$$

The term $k = 0$ gives the leading diverging term in the limit $\epsilon \to 0$, and so the sum can be rewritten as

$$S_n = \frac{\pi^2}{24\epsilon} \left(1 + \frac{1}{n}\right) + \frac{\ln 2}{2} + \frac{1}{1-n} \sum_{k=1}^{\infty} \left[\frac{n}{2k} \text{csch} \frac{\pi^2 k}{\epsilon} - \frac{1}{2k} \text{csch} \frac{\pi^2 k}{\epsilon n} \right] \,, \tag{19}$$

where the leftover sum over k is vanishing in the limit $\epsilon \to 0$. This equation is exact for any ϵ as it is Eq. (12) from which we started and it is just another expansion of the elliptic function found in Ref. [17]. However, in this form S_n is ready for the asymptotic expansion close to $\epsilon = 0$. For small ϵ, we have

$$\text{csch} \frac{\pi^2 k}{\epsilon n} \simeq 2 \exp(-\frac{\pi^2 k}{\epsilon n}) \,. \tag{20}$$

Using Eq. (11), we have that each of these terms gives a correction of the form

$$\exp(-\frac{\pi^2 k}{\epsilon n}) \simeq \xi^{-2k/n} \,. \tag{21}$$

These subleading corrections clearly depend on the precise definition used for the correlation length. Thus the universal character is only in the exponents $2k/n$, the amplitudes being normalization dependent. These corrections agree with the scaling form proposed in the introduction with $x = 2$. However, for the gapless case a multiplicative logarithmic correction is also introduced by a marginal operator [21], but it does not appear in the gapped phase. This result agrees with the recent ones in Ref. [22].

2.2. Other models

Several other models can be treated with the help of CTMs and the same procedure as above for the XXZ model applies. This generalization is made particularly simple by the fact that in the considered cases the only change is the expression of ϵ_j as function of the Hamiltonian parameters.

The most studied example is the Ising model in a transverse magnetic field with Hamiltonian

$$H_I = -\sum_j \left[\sigma_j^x \sigma_{j+1}^x + h\sigma_j^z\right] . \tag{22}$$

This models displays a quantum critical point at $h = 1$ separating a ferromagnetic phase ($h < 1$) from a quantum paramagnetic one ($h > 1$). Rényi entropies for this model have been already calculated in Ref. [17] and so the following results are not new, but just an asymptotic expansion of known expressions.

The "single-particle levels" of the resulting $H_{\rm CTM}$ are [13]

$$\epsilon_j = \begin{cases} (2j+1)\epsilon & \text{for } h > 1\,, \\ 2j\epsilon & \text{for } h < 1\,, \end{cases} \qquad \text{with } \epsilon = \pi \frac{K(\sqrt{1-k^2})}{K(k)}\,, \tag{23}$$

where $K(k)$ is the complete elliptic integral of the first kind [23], and $k = \min[h, h^{-1}]$. An expression for the correlation length is exactly known [10], but for what follows we are only interested in the behavior close to the critical point

$$\ln \xi = \frac{\pi^2}{\epsilon} + O(\epsilon^0)\,, \tag{24}$$

valid in both phases.

In the ferromagnetic phase $h < 1$, the dependence of ϵ_j on j is the same as in the XXZ model, only ϵ is different. Thus Eq. (19) is valid also for the Ising model. When plugging Eq. (24) into this expression, we get a leading term corresponding to the central charge $c = 1/2$ and corrections going like $\xi^{-k/n}$, in agreement with the presence of the energy operator of dimension $x = 1$ as in the conformal case [6, 8].

In the paramagnetic phase $h > 1$, the calculation is equivalent with the difference that the generalized Poisson resummation formula

$$\sum_{j=-\infty}^{\infty} f(|\epsilon(bj+a)|) = \frac{2}{\epsilon b} \sum_{k=-\infty}^{\infty} \hat{f}\left(\frac{2\pi k}{\epsilon b}\right) e^{2\pi i k a/b}\,, \tag{25}$$

must be used. From Eq. (23), we can choose $a = 1/2$ and $b = 1$ (or any multiple by changing the definition of $f(x)$). The starting formula is

$$\begin{aligned} S_n &= \frac{1}{1-n} \sum_{j=0}^{\infty} \left(f_n(\epsilon(j+1/2)) - n f_1(\epsilon(j+1/2))\right) \\ &= \frac{1}{2}\frac{1}{1-n} \sum_{j=-\infty}^{\infty} \left(f_n(|\epsilon(j+1/2)|) - n f_1(|\epsilon(j+1/2)|)\right)\,, \end{aligned} \tag{26}$$

where we notice the absence of the additive $\ln 2$ term (connected with a non-degenerate ground state). Thus, after Poisson resumming we have

$$S_n = \frac{1}{1-n} \sum_{k=-\infty}^{\infty} (-1)^k \left[\frac{n}{4k} \mathrm{csch} \frac{\pi^2 k}{\epsilon} - \frac{1}{4k} \mathrm{csch} \frac{\pi^2 k}{\epsilon n}\right] . \tag{27}$$

where the main difference compared to the previous case is the factor $(-1)^k$. Thus in the expansion in terms of the correlation length ξ the same power-laws enter but with alternating amplitudes.

A particular simple further generalization is the XY chain for which all the formulas above are the same (see e.g. [24]) and only the expression of k in terms of the h and γ changes according to

$$k = \begin{cases} \sqrt{h^2+\gamma^2-1}/\gamma & \text{for}\, h>1\,, \\ \gamma/\sqrt{h^2+\gamma^2-1} & \text{for}\, h<1\,, \end{cases} \tag{28}$$

valid for $\gamma^2 + h^2 > 1$. This is reminiscent of the fact that at $h = 1$ the transition is always in the Ising universality class and a simple rescaling can absorb the values of γ. Physically more interesting is the limit $h = 0$, not included in the case above, but with CTMs known [10]. One has $\epsilon_j = j\epsilon$ and $k = (1-\gamma)/(1+\gamma)$. The derivation of S_n is straightforward and one recovers the same corrections as for the Ising model, with a doubled leading term reflecting the values of the central charge $c = 1$. This is connected also to an exact relation between Ising and XX models [25].

Also XYZ chains (see [26] for S_1) and spin $\kappa/2$ analogue of the XXZ quantum spin chain (see [20] for S_1) can be simply obtained from the formulas above.

2.3. The single-copy entanglement

The limit $n \to \infty$ requires a separated analysis, because in Eq. (5) the exponent of the corrections goes to zero, signaling the appearance of logarithmic corrections to the scaling as for the conformal case. S_∞ is called single copy entanglement [27, 28, 19] and it is obtained by taking the limit $n \to \infty$ before the limit $\epsilon \to 0$, since the two do not commute. It is easy to get the logarithmic corrections exactly. For $n \to \infty$, Eq. (19) becomes

$$S_\infty = \frac{\pi^2}{24\epsilon} + \frac{\ln 2}{2} + \sum_{k=1}^{\infty}\left[\frac{\epsilon}{2\pi^2 k^2} - \frac{1}{2k}\text{csch}\frac{\pi^2 k}{\epsilon}\right] \tag{29}$$

$$= \frac{\pi^2}{24\epsilon} + \frac{\ln 2}{2} + \frac{\epsilon}{12} - \sum_{k=1}^{\infty}\frac{1}{2k}\text{csch}\frac{\pi^2 k}{\epsilon}\,. \tag{30}$$

The left over sum gives standard power-law corrections and they do not involve 'unusual' exponents. The unusual part is in the logarithmic corrections encoded in the term $\epsilon/12$. Indeed using $\ln\xi = \pi^2/(a\epsilon)$ (with $a = 1$ for Ising ferromagnetic and $a = 2$ for XXZ), we have

$$S_\infty - S_\infty^{\text{asy}} \simeq \frac{\pi^2}{12a\log\xi}. \tag{31}$$

Notice that when written in terms of ϵ this expression has a unique correction, that is particularly simple for the XXZ chain since $\epsilon = \text{arccosh}\Delta$.

For the Ising model in the paramagnetic phase $h > 1$, the terms $(-1)^k$ change the $1/\epsilon$ term, and the final result is

$$S_\infty = \frac{\pi^2}{24\epsilon} - \frac{\epsilon}{24} - \sum_{k=1}^{\infty}\frac{(-1)^k}{2k}\text{csch}\frac{\pi^2 k}{\epsilon}\,. \tag{32}$$

Notice that the amplitudes of the corrections are different in the two phases and their numerical values are of the same form of what found for the critical XX spin-chain [8]. These results for the single copy entanglement in XY chains have been reported also in [19, 28].

3. Relation to Virasoro characters

The above examples may be considered as special cases of a more general phenomenon: that in many integrable models satisfying the Yang-Baxter relations, traces of powers of the CTM may be expressed in terms of the Virasoro characters of the corresponding CFT of the critical theory. These enjoy simple properties under modular transformations which allow us to extract the 'unusual' corrections to scaling discussed earlier.

To be specific, the Boltzmann weights of many integrable models lie on a curve specified by an elliptic modulus q, where the critical point corresponds to $q \to 1$. The examples of quantum spin chains considered above correspond to $q = e^{-2\epsilon}$. Baxter [10] showed that in these models the eigenvalues of the 4th power $\hat{A}^4$ of the CTM are all of the form q^{aN+b}, for integer $N \geq 0$, with a computable degeneracy d_N. It was then observed in the late 1980s (see, for example, Refs. [29, 30]) that the degeneracy factors are just those appearing in the highest weight representations of the Virasoro algebras in the CFT which describes the scaling limit at the critical point, that is

$$\chi_\Delta(q) = q^{-c/24+\Delta} \sum_{N=0}^{\infty} d_N q^N \,, \tag{33}$$

where c is the central charge and Δ is the highest weight of the representation, giving the dimension $x = 2\Delta$ of a scaling operator of the theory. The value of Δ depends on the value of the spin at the origin, and the boundary conditions at infinity. This observation, although not proven in general, was based on the facts that (a) in the scaling limit at the critical point, but in a finite annulus with outer and inner radii $R_>$ and $R_<$, the eigenvalues of the CTM have precisely this form, with conjugate modulus $\tilde{q}$ (defined below) equal to $R_</R_>$ – this follows from boundary CFT [31]; and (b) in the integrable RSOS models, the eigenstates of the CTM correspond to a semi-infinite walk on the corresponding A_m diagram, and the Virasoro generators act simply on the space of these paths. (In fact it was shown by the Kyoto group [32] that for higher integrable models obtained by fusion the result is not always a simple character but rather a branching coefficient of an affine algebra. However these still enjoy simple modular properties as described below.)

This means, in particular, that the partition function $\mathrm{Tr}\,\hat{A}^4$ is proportional to $\chi_\Delta(q^a)$ for some Δ (which depends on, for example, which massive phase the model is in). Without loss of generality we take $a = 1$. In general the partition function may be a linear combination of characters, depending on the choice of boundary conditions at the origin and infinity. This complicates the argument without changing the general conclusion, and we shall assume that the boundary conditions are such as to pick out a single character, as in the examples discussed earlier. However we remark that, in the context of entanglement entropy, we should specify if we fix the spin at the origin in the direct or in the dual lattice. In all examples above, we fixed the dual variable, by leaving the bond between the two halves free. However, while at first it could sound strange, also fixing an actual spin at the origin makes sense for the entanglement entropy, because in the CTM this does not correspond to fixing it in the hamiltonian (which would effectively divide the chain into two non-interacting halves). Rather it means projecting the ground state $|0\rangle$ into a subspace in which the spin at the origin is fixed, and measuring the entanglement between the two halves of the chain in this subspace. Thus we expect to be able to explore other values of Δ by such a procedure, and will therefore keep it general in what follows.

The point now is that the trace of $\hat{A}^{4n}$ is, in the basis in which the CTM is diagonal, given simply by replacing $q \to q^n$, and thus

$$\mathrm{Tr}\,\rho_{\mathcal{A}}^n = \frac{\chi_\Delta(q^n)}{\big(\chi_\Delta(q)\big)^n}\,. \tag{34}$$

We are interested in the limit $q \to 1$ close to the critical point, where the series expressions (33) for $\chi_\Delta(q)$ are not very useful. However [33], the Virasoro characters transform linearly under a modular transformation $q \to \tilde{q}$, where, if $q = e^{-2\epsilon}$, $\tilde{q} = e^{-2\pi^2/\epsilon}$:

$$\chi_\Delta(q) = \sum_{\Delta'} S_\Delta^{\Delta'} \chi_{\Delta'}(\tilde{q})\,, \tag{35}$$

where $S_\Delta^{\Delta'}$ is the modular S-matrix which characterizes the CFT. Notice that the modular invariance plays exactly the same rule as Poisson resummation above, but it is more general.

As $q \to 1$, $\tilde{q} \to 0$, so it is straightforward to extract the leading behavior and all the corrections. The leading term comes from $\Delta' = 0$, in which case we see that

$$\mathrm{Tr}\,\rho_{\mathcal{A}}^n \sim \left(S_\Delta^0\right)^{1-n} \left(\tilde{q}^{-c/24}\right)^{n^{-1}-n}\,,$$

which gives

$$S_n \sim -\frac{c}{24}\left(1+\frac{1}{n}\right)\ln\tilde{q} + \ln\left(S_\Delta^0\right) + o(1)\,. \tag{36}$$

Comparing with (4), we see that $\tilde{q} \propto \xi^{-2}$. The $O(1)$ term is related to the Affleck-Ludwig boundary entropy [34] $g_\Delta = \ln\left(S_\Delta^0\right)^{1/2}$. Note that we get twice the boundary entropy because there are two semi-infinite chains adjoining the spin at the origin. The examples discussed earlier presumably correspond to $\Delta = 0$ and the corresponding $O(1)$ term can be absorbed into the non-universal constant of proportionality between $\tilde{q}$ and ξ^{-2}.

The corrections now come from (a) integer powers of $\tilde{q}$, that is powers of ξ^{-2}, in the expansion of the character, and (b) other characters with $\Delta' > 0$. The leading terms of the latter form then give rise to corrections to (36)

$$(1-n)^{-1}\sum_{\Delta'>0}\frac{S_\Delta^{\Delta'}}{S_\Delta^0}\left(\tilde{q}^{\Delta'/n} - n\tilde{q}^{\Delta'}\right) + \cdots\,. \tag{37}$$

(The second power is less important for $n > 1$ but is included so as to ensure the finiteness as $n \to 1$.) Recalling that $2\Delta' = x'$, we see that we get corrections of the form $\xi^{-x'/n}$ as expected. However, unless the matrix element $S_\Delta^{\Delta'}$ happens to vanish, in principle we get such contributions from *all* the scaling dimensions x' of primary fields, not just the relevant ones. Also, the higher order corrections in general involve powers which are all possible integer linear combinations of x'/n and x'. The evidence of these further corrections has been reported for simple gapless spin chains [8], but it would be as interesting to report them in the gapped case.

We can also derive a general result for the single-copy entanglement S_∞. Using Eq. (34) we see that

$$S_\infty = -(-c/24 + \Delta)\ln q + \ln\chi_\Delta(q)\,. \tag{38}$$

The second term, after using the modular transformation, goes like $(-c/24+\Delta')\log\tilde{q}$ plus power-law corrections. We expect the leading term in the sum over Δ' to come from $\Delta'=0$. Thus we get a universal term $(c/12)\ln\xi$. This corresponds to the first term in Eqs. (30) and (32). The first term in Eq. (38) gives the 'unusual' correction discussed in Sec. 2.3. Since $\tilde{q}\propto\xi^{-2}$, $\ln q\sim -2\pi^2/\ln\xi$, so this correction has the form

$$\frac{2\pi^2(-c/24+\Delta)}{\ln\xi}\,. \tag{39}$$

This agrees with the Ising case in the ferromagnetic phase given by Eq. (31) using $c=1/2$, $\Delta=1/16$, and in the paramagnetic Eq. (32) using $c=1/2$ and $\Delta=0$.

4. Concluding remarks

We showed that the corrections to the scaling of the Rényi entanglement entropies in gapped systems display the universal form (5) in the case when an infinite line is divided into two semi-infinite subsystems. We provided few explicit examples using known corner transfer matrices and we argue that in the general case these corrections are a consequence of the modular invariance of the traces of powers of the CTM when expressed in terms of the Virasoro characters.

This result generalizes straightforwardly to more complicated bipartitions provided the correlation length ξ is smaller than all separations. Eq. (5) only gets multiplied by the number of boundary points between $\mathcal{A}$ and $\mathcal{B}$. The rigorous result for a finite interval of length ℓ obtained for the XY model [17] confirms this. However, for a finite interval, only when ℓ becomes much larger than ξ, the asymptotic behavior would be visible. For smaller values of ℓ, a complicated crossover between the conformal result and the asymptotic one takes place as already known for the leading terms [35]. The characterization of all these corrections is not only an academic task. In the case of the entanglement of two disjoint intervals in a conformal model, their precise knowledge has been fundamental to recover the CFT predictions [36, 37] in numerical calculations [38, 39, 40, 41]. We believe that the same is true for massive systems, especially in the case of non-integrable models when numerical calculations are the only way to attack the problem. A final question is whether these unusual corrections are also present for other entanglement measures that displayed them in the gapless phases as the valence bond entanglement [42], and if yes whether it is possible to calculate them exactly.

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